Notes for AA214, Chapter 12 SPLIT AND FACTORED FORMS

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Introduction

- 1. Factored forms of numerical operators are used extensively in constructing and applying numerical methods to problems in fluid mechanics.
- 2. Concepts such as: "hybrid", "time split", and "fractional step" methods.
- 3. Especially useful for the derivation of practical algorithms that use implicit methods.

Concepts

- 1. Concept 1: Matrices can be split in quite arbitrary ways.
- 2. Concept 2: Advancing to the next time level always requires some reference to a previous one.
- 3. Concept 3: Time marching methods are valid only to some order of accuracy in the step size, h.

Splitting

1. Starting with:

$$\frac{d\vec{u}}{dt} = A\vec{u} - \vec{f} \tag{1}$$

2. Consider arbitrary splitting of A, Concept 1:

$$\frac{d\vec{u}}{dt} = [A_1 + A_2]\vec{u} - \vec{f} \tag{2}$$

where $A = [A_1 + A_2]$, but A_1 and A_2 are not unique.

1^{st} order Explicit Splitting

- 1. Choose the simple, first-order, a explicit Euler method.
- 2. New data \vec{u}_{n+1} in terms of old \vec{u}_n Concept 2:

$$\vec{u}_{n+1} = [I + hA_1 + hA_2]\vec{u}_n - h\vec{f} + O(h^2)$$
(3)

3. Equivalently:

$$\vec{u}_{n+1} = [[I + hA_1][I + hA_2] - h^2A_1A_2]\vec{u}_n - h\vec{f} + O(h^2)$$

^aSecond-order time-marching methods are considered later.

4. Finally, from Concept 3: (allowing us to drop higher order terms):

$$\vec{u}_{n+1} = [I + hA_1][I + hA_2]\vec{u}_n - h\vec{f} + O(h^2)$$
(4)

- 5. Eqs. 3 and 4 have the same formal order of accuracy
- 6. Neither one is to be preferred over the other.
- 7. However, their numerical stability can be quite different
- 8. Also, techniques to carry out their numerical evaluation can have arithmetic operation counts that vary by orders of magnitude.

Factoring Physical Representations: Time Splitting

1. PDE representing: convection A_c and dissipation A_d .

$$\frac{d\vec{u}}{dt} = A_c \vec{u} + A_d \vec{u} + (\vec{bc}) \tag{5}$$

2. Euler Explicit

$$\vec{u}_{n+1} = [I + hA_d + hA_c]\vec{u}_n + h(\vec{bc}) + O(h^2)$$
(6)

- 3. Factoring the dissipation term and the convection term produces a two step process
- 4. Results in additional error and possible stability consequences.

5. Factored form

$$\vec{u}_{n+1} = [I + hA_d] \Big([I + hA_c] \vec{u}_n + h(\vec{bc}) \Big)$$

$$= \underbrace{[I + hA_d + hA_c] \vec{u}_n + h(\vec{bc})}_{\text{Original Unfactored Terms}}$$

$$+ \underbrace{h^2 A_d \Big(A_c \vec{u}_n + (\vec{bc}) \Big)}_{\text{Higher-Order Terms}} + O(h^2)$$

$$(7)$$

- 6. Eq. 7 and the original unfactored form Eq. 6 have identical orders of accuracy in the time approximation.
- 7. Apply a predictor-corrector sequence.

$$\tilde{u}_{n+1} = [I + hA_c]\tilde{u}_n + h(\vec{bc})$$

$$\vec{u}_{n+1} = [I + hA_d]\tilde{u}_{n+1} \tag{8}$$

Implicit-Explicit Factoring

- 1. Split combinations of implicit and explicit techniques.
- 2. Apply a partially implicit-explicit method to Eq. 5

$$\vec{u}_{n+1} = [I + hA_c]\vec{u}_n + hA_d\vec{u}_{n+1} + h(\vec{bc}) + O(h^2)$$
(9)

3. Rewrite as:

$$\vec{u}_{n+1} = [I - hA_d]^{-1} \Big([I + hA_c]\vec{u}_n + h(\vec{bc}) \Big)$$

$$= \underbrace{[I + hA_d + hA_c]\vec{u}_n + h(\vec{bc})}_{\text{Original Unfactored Terms}} + O(h^2) \tag{10}$$

4. Using

$$[I - hA_d]^{-1} = I + hA_d + h^2 A_d^2 + \cdots$$

if $h \cdot ||A_d|| < 1$, where $||A_d||$ is some norm of $[A_d]$.

5. A predictor-corrector interpretation leads to the sequence

$$\tilde{u}_{n+1} = [I + hA_c]\vec{u}_n + h(\vec{bc})$$

$$[I - hA_d]\vec{u}_{n+1} = \tilde{u}_{n+1} \tag{11}$$

- 6. The diffusion operator is now implicit, requiring a tridiagonal solver if the diffusion term is central differenced.
- 7. Numerical stiffness is generally much more severe for the diffusion process, this factored form would appear to be superior to that provided by Eq. 8. **But, Stability?**

Factoring Space Matrix Operators in 2–D

- 1. Physical systems are inherently multidimensional
- 2. Three-Dimensional (3D) Wave equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} + b \frac{\partial u}{\partial y} + c \frac{\partial u}{\partial z} = 0$$

3. Two-Dimensional (2D) Diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

4. Navier-Stokes equations

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = 0$$

Mesh Indexing Convention

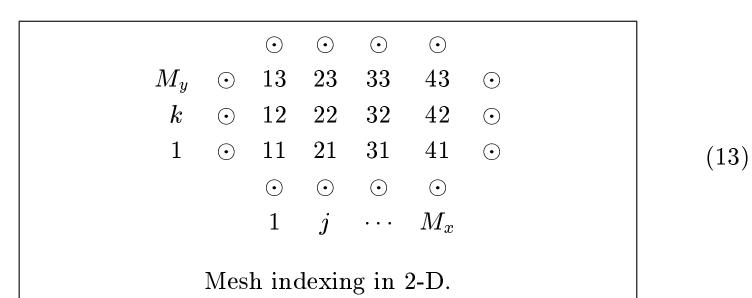
1. Linear 2-D scalar PDE that models diffusion:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \tag{12}$$

- 2. Reduce PDE to a coupled set of ODE's by differencing the space derivatives on a mesh (graph, net).
- 3. Inspecting the resulting matrix operator.

Mesh Indexing

1. Assume a 3×4 point mesh^a



^aThis could also be called a 5×6 point mesh if the boundary points (labeled \odot in the sketch) were included, here we just consider interior points.

- 2. $M_x = 4$, the number of (interior) x points
- 3. $M_y = 3$, the number of (interior) y points
- 4. The numbers $11, 12, \dots, 43$ represent the location in the mesh of the dependent variable bearing that index.
- 5. Thus u_{32} represents the value of u at j=3 and k=2.
- 6. NOTE: This notation assume we order the points with the j or x index first and the k or y index second.

Data-Bases and Space Vectors

- 1. DATA-BASE: dimensioned array in a computer code that allots the storage locations of the dependent variable(s)
- 2. Many ways to lay out a data-base.
- 3. Consider only two:
 - (a) (x)-vectors: consecutively along rows that are themselves consecutive from k = 1 to M_y
 - (b) (y)-vectors: Consecutively along columns that are consecutive from j = 1 to M_x .
- 4. Refer to each row or column group as a *space vector* (they represent data along lines that are continuous in space)
- 5. Label their sum with the symbol U.

- 6. To be specific about the structure
 - (a) Label a data-base composed of x-vectors with $U^{(x)}$
 - (b) Example: $U^{(x)} = (u_{11}, u_{21}, u_{31}, u_{41}, u_{12}, u_{22}, u_{32}, u_{42}, u_{13}, u_{23}, u_{33}, u_{43})^T$
 - (c) Label a data-base composed of y-vectors with $U^{(y)}$.
 - (d) Example: $U^{(y)} = (u_{11}, u_{12}, u_{13}, u_{21}, u_{22}, u_{23}, u_{31}, u_{32}, u_{33}, u_{41}, u_{42}, u_{43})^T$

Data-Base Permutations

1. Two vectors (arrays) are related by a permutation matrix P:

$$U^{(x)} = P_{xy}U^{(y)}$$
 and $U^{(y)} = P_{yx}U^{(x)}$ with $P_{yx} = P_{xy}^T = P_{xy}^{-1}$ (1)

- 2. Consider the structure of a matrix finite-difference operator representing 3-point central-differencing schemes for both space derivatives in two dimensions.
- 3. When the matrix is multiplying a space vector U, the usual (but ambiguous) representation is given by A_{x+y} .

$$\frac{dU}{dt} = A_{x+y}U + (\vec{bc}) \tag{15}$$

4. If it is important to be specific about the data-base structure, we use the notation $A_{x+y}^{(x)}$ or $A_{x+y}^{(y)}$, depending on the data-base chosen for the U it multiplies.

Example for $U^{(x)}$ Ordering

- 1. Data-base composed of M_y x-vectors stored in $U^{(x)}$.
- 2. Entries for $x \to x$, for $y \to o$, for both $\to \bullet$.

Example for $U^{(y)}$ Ordering

- 1. Data-base composed of M_x y-vectors stored in $U^{(y)}$.
- 2. Entries for $x \to x$, for $y \to o$, for both $\to \bullet$.

Permutation Discussion

- 1. Notice that the matrices are not the same although they represent the same derivative operation.
- 2. Their structures are similar, however, and they are related by the same permutation matrix that relates $U^{(x)}$ to $U^{(y)}$.

$$A_{x+y}^{(x)} = P_{xy} \cdot A_{x+y}^{(y)} \cdot P_{yx} \tag{18}$$

Space Splitting and Factoring: (x) Ordering

1. The matrix $A_{x+y}^{(x)}$ can be split into two matrices such that

$$A_{x+y}^{(x)} = A_x^{(x)} + A_y^{(x)} (19)$$

Space Splitting and Factoring: (y) Ordering

1. Similarly

$$A_{x+y}^{(y)} = A_x^{(y)} + A_y^{(y)} (22)$$

Matrix Relations: Permutations

1. The permutation relation also holds for the split matrices, so

$$A_y^{(x)} = P_{xy} A_y^{(y)} P_{yx}$$

and

$$A_x^{(x)} = P_{xy} A_x^{(y)} P_{yx}$$

2. The splittings can be combined with factoring

Example

1. First-order in time:implicit Euler method

$$U_{n+1}^{(x)} = U_{n}^{(x)} + h \left[A_{x}^{(x)} + A_{y}^{(x)} \right] U_{n+1}^{(x)} + h(\vec{bc})$$

$$\left[I - hA_x^{(x)} - hA_y^{(x)}\right]U_{n+1}^{(x)} = U_n^{(x)} + h(\vec{bc}) + O(h^2)$$
(25)

2. Retain first-order accuracy with the alternative

$$\left[I - h A_{x}^{(x)}\right] \left[I - h A_{y}^{(x)}\right] U_{n+1}^{(x)} = U_{n}^{(x)} + h(\vec{bc}) + O(h^{2})$$
(26)

3. Predictor-corrector form and permute the data-base of the second row.

$$\begin{bmatrix} I - h A_x^{(x)} \end{bmatrix} \tilde{U}^{(x)} = U_n^{(x)} + h(\vec{bc})$$

$$\begin{bmatrix} I - h A_y^{(y)} \end{bmatrix} U_{n+1}^{(y)} = \tilde{U}^{(y)}$$
(27)

Second-Order Factored Implicit Methods

- 1. Second-order accuracy in time can be maintained
- 2. Trapezoidal method where the derivative operators have been split

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]U_{n+1} =$$

$$\left[I + \frac{1}{2}hA_x + \frac{1}{2}hA_y\right]U_n + h(\vec{bc}) + O(h^3)$$
(28)

3. Factor both sides giving

$$\left[\left[I - \frac{1}{2} h A_x \right] \left[I - \frac{1}{2} h A_y \right] - \frac{1}{4} h^2 A_x A_y \right] U_{n+1}
= \left[\left[I + \frac{1}{2} h A_x \right] \left[I + \frac{1}{2} h A_y \right] - \frac{1}{4} h^2 A_x A_y \right] U_n +
h(\vec{bc}) + O(h^3)$$
(29)

4. Note that the combination $\frac{1}{4}h^2[A_xA_y](U_{n+1}-U_n)$ is proportional to h^3 : since $(U_{n+1}-U_n)$ is proportional to h.

$$\left[I - \frac{1}{2}hA_x\right] \left[I - \frac{1}{2}hA_y\right] U_{n+1} =
\left[I + \frac{1}{2}hA_x\right] \left[I + \frac{1}{2}hA_y\right] U_n + h(\vec{bc}) + O(h^3)$$

- 5. Both the factored and unfactored form of the trapezoidal method are second-order accurate in the time march.
- 6. An alternative form of this kind of factorization is the classical ADI (alternating direction implicit) method

$$\left[I - \frac{1}{2}hA_x\right]\tilde{U} = \left[I + \frac{1}{2}hA_y\right]U_n + \frac{1}{2}hF_n
\left[I - \frac{1}{2}hA_y\right]U_{n+1} = \left[I + \frac{1}{2}hA_x\right]\tilde{U} + \frac{1}{2}hF_{n+1} + O(h^3)$$

Importance of Factored Forms: 2D and 3D

- 1. Time-march equations are stiff, and implicit methods are required to permit reasonably large time steps
- 2. The use of factored forms becomes a very valuable tool for realistic problems.
- 3. Consider,

$$\[I - \frac{1}{2}hA_{x+y}\]U_{n+1} = \left[I + \frac{1}{2}hA_{x+y}\right]U_n + h(\vec{bc})$$

- 4. M_x number of points in x, M_y number of points in y
- 5. Accumulate the right-hand-side in the array (RHS).

6. Solving for U_{n+1} requires the solution of a sparse, but very large, set of coupled simultaneous equations, e.g.,

- 7. In real cases involving the 2-D Euler or Navier-Stokes equations, each symbol (o, x, \bullet) represents a 4×4 block matrix with entries that depend on the pressure, density and velocity field, $(5 \times 5 \text{ in } 3D)$.
- 8. Suppose we were to solve the equations directly.
- 9. The forward sweep of a simple Gaussian elimination fills all of the 4×4 blocks between the main and outermost diagonal,

- 10. This must be stored in computer memory to be used to find the final solution in the backward sweep.
- 11. If N_e represents the order of the small block matrix (4 in the 2-D Euler case), the approximate memory requirement is

$$(N_e \times M_y) \cdot (N_e \times M_y) \cdot M_x$$

floating point words.

- 12. Here it is assumed that $M_y < M_x$. If $M_y > M_x$, M_y and M_x would be interchanged.
- 13. A moderate mesh of 60×200 points would require over 11 million words to find the solution.
- 14. The next consideration is operation counts for the solution process.
- 15. A full matrix of rank (size) N requires $O(N^3)$ floating point operations (FLOP)to solve the linear system.

- 16. A matrix with band width b^{a} requires $O(Nb^{2})$ FLOP
- 17. The 2D example would then require $O((N_e \cdot M_x \cdot M_y) \cdot Min(N_e \cdot M_x, N_e \cdot M_y)^2)$ FLOP
- 18. The 60×200 point example would require $\approx 10^9$ FLOP
- 19. In a practical application, each iteration n requires the large sparse linear solve with typically 10^3 to 10^4 times steps, leading to $\approx 10^{12} 10^{13}$ FLOP per case.
- 20. With computing speeds of over one teraflop,^b direct solvers may become useful for finding steady-state solutions of practical problems in two dimensions.

^aBand width b, is defined as the maximum number of off diagonals with non-zero entries plus one for the center diagonal. For example: a tridiagonal matrix has b=2, a pentra-diagonal matrix b=3

^bOne trillion floating-point operations per second.

21. However, a three-dimensional solver would require a memory of approximately

$$N_e^2 \cdot M_y^2 \cdot M_z^2 \cdot M_x$$

words, and, for well resolved flow fields, this probably exceeds memory availability for some time to come.

- 22. Operation counts for a direct solver in 3D c are in the $> 10^{16}$ range
- 23. On the other hand, consider computing a solution using the factored implicit equation

$$\left[I - \frac{1}{2}hA_x\right] \left[I - \frac{1}{2}hA_y\right] U_{n+1} =
\left[I + \frac{1}{2}hA_x\right] \left[I + \frac{1}{2}hA_y\right] U_n + h(\vec{bc})$$

24. Again, form the (RHS)

^cA 4 million point grid: $M_x = 100, M_y = 200, M_z = 200, N_e = 5$

25. Write the remaining terms in the two-step predictor-corrector form

$$\left[I - \frac{1}{2}hA_x^{(x)}\right]\tilde{U}^{(x)} = (RHS)^{(x)}
\left[I - \frac{1}{2}hA_y^{(y)}\right]U_{n+1}^{(y)} = \tilde{U}^{(y)}$$
(30)

- 26. First step: solved using M_y uncoupled block tridiagonal solvers^d.
- 27. This is equivalent to solving M_y one-dimensional, 1-D problems, each with M_x blocks of order N_e .

28. Temporary solution $\tilde{U}^{(x)}$ would then be permuted to $\tilde{U}^{(y)}$

^dA block tridiagonal solver is similar to a scalar solver except that small block matrix operations replace the scalar ones, and matrix multiplications do not commute.

29. Next step: solve M_x 1D implicit problems each with dimension M_y .

- 30. The band width for both steps is now $b = 2N_e$
- 31. An Operation count for each step is: $M_y \times M_x \times 4 \times N_e^2$

- 32. In the 60×200 example the total is : $\approx 2 \times 10^6$ FLOP per time step
- 33. Significantly less than the direct solve, $\approx 3 \times 10^9$ FLOP per time step
- 34. In 3D the savings are even more significant.
- 35. For example, in the shuttle analysis: $(20 \times 10^6 \text{ grid points})$
 - (a) $\approx 10^{18}$ FLOP per time step for direct solve
 - (b) $\approx 10^{10}$ FLOP per time step for the 3 block tridiagonals solves

The Delta Form

- 1. There are many ways can be devised to split the matrices and generate factored forms.
- 2. An especially useful form for ensuring a correct steady-state solution in a converged time-march: "delta form,"
- 3. Consider the unfactored form of the trapezoidal method

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]U_{n+1} =
\left[I + \frac{1}{2}hA_x + \frac{1}{2}hA_y\right]U_n + h(\vec{bc}) + O(h^3)$$
(31)

4. From both sides subtract

$$\left[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y\right]U_n$$

5. Define: $\Delta U_n = U_{n+1} - U_n$, and rewritting

$$\[I - \frac{1}{2}hA_x - \frac{1}{2}hA_y \] \Delta U_n = h \left[A_{x+y}U_n + (\vec{bc}) \right] + O(h^3) \quad (32)$$

- 6. Note: the right side of this equation is the product of h and a term that is identical to the right side of our original ODE.
- 7. Thus, if Eq. 32 converges, it is guaranteed to converge to the correct steady-state solution of the ODE.
- 8. Factor Eq. 32 maintaining second-order accuracy

$$\[I - \frac{1}{2}hA_x\] \left[I - \frac{1}{2}hA_y\] \Delta U_n = h\left[A_{x+y}U_n + (\vec{bc})\right] + O(h^3) \quad (33)$$

- 9. This is the delta form of a factored, second-order, 2-D equation.
- 10. In spite of the similarities in derivation between the non- "delta" and "delta" form, the convergence properties are vastly different.